2,2-Bis(bromomethyl)-1,3-propanediol
3296-90-0 | DTXSID9020164

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 104 °C

Global applicability domain: Inside

Local applicability domain index: 6.61e-01

Confidence level: 6.19e-01

Nearest Neighbors from the Training Set

Image not found
2,2-Bis(bromomethyl)-1,3-propanediol
Measured: 113
Predicted: 104

Image not found
Loprodiol
Measured: 83.0
Predicted: 87.0

Image not found
3-Iodo-1,2-propanediol
Measured: 48.5
Predicted: 56.7

Image not found
Chlorphenesin
Measured: 78.0
Predicted: 79.3